Bioinformatics study on the role of aromatic amino acids in the position of residue Leucine 25 in Aequorin with site-directed mutagenesis

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Abstract: Ca^{2+}-regulated photoproteins are single-chain proteins showing high homology in aspect of amino acid sequences. They contain three EF-hand Ca^{2+}-binding loops. Aequorin is one of the calcium-regulated photoproteins, which is capable of producing light in the presence of coelenterazine substrates, molecular oxygen, and calcium initiator. The Leucine 25 is one of the residues of EF-hand I, and the fourth residue in the cavity of coelenterazine. The effect of replacement of aromatic residues including phenylalanine, tyrosine and tryptophan in the position of Leucine 25 on aequorin function has been investigated. For this purpose, the mutation model was designed using Moderller 9v19 software and the best model was selected using software of ModEval, SAVES, SPdbViewer and PIC Server. Moreover, the status of biochemical-physical properties of the wildtype proteins and mutants were investigated. The 3D structure of the mutants was also plotted by the Chimera software. The results showed that applying the 3 mutations in the position of Leucine 25 reduced the structural stability of aequorin.

Keywords: Aequorin; Site-directed mutagenesis; Photoprotein; Calcium; Coelenterazine.

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